

L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, isoheptyl ester

Inchi:	InChI=1S/C20H25F6NO3/c1-11(2)6-5-9-30-18(29)16(12(3)4)27-17(28)14-10-13(19(21,22)20)
InchiKey:	UCIXFVGHQYSETG-UHFFFAOYSA-N
Formula:	C20H25F6NO3
SMILES:	CC(C)CCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]:	441.41

Physical Properties

Property code	Value	Unit	Source
gf	-1233.28	kJ/mol	Joback Method
hf	-1756.45	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.458		Crippen Method
mvol	298.510	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	861.81	K	Joback Method
tc	1058.39	K	Joback Method
tf	504.75	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.24	J/molxK	861.81	Joback Method
cpg	968.26	J/molxK	894.57	Joback Method
cpg	981.29	J/molxK	927.34	Joback Method
cpg	993.38	J/molxK	960.10	Joback Method
cpg	1004.61	J/molxK	992.86	Joback Method
cpg	1015.03	J/molxK	1025.63	Joback Method
cpg	1024.73	J/molxK	1058.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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